Droplets in the coexistence region of the two-dimensional Ising model

M Pleimling§† and   W Selke§

§ Institut für Theoretische Physik, Technische Hochschule, D–52056 Aachen, Germany
† Institut für Theoretische Physik 1, Universität Erlangen-Nürnberg, D–91058 Erlangen, Germany

Abstract. The two–dimensional Ising model with fixed magnetization is studied using Monte Carlo techniques. At the coexistence line, the macroscopic, extensive droplet of minority spins becomes thermally unstable by breaking up into microscopic clusters. Intriguing finite–size effects as well as singularities of thermal and cluster properties associated with the transition are discussed.

Short title: Droplets in Ising model

February 1, 2008

The two–dimensional Ising model has attracted much interest in the past. It is conceptually simple, and several of its non–trivial properties can be determined exactly [1]. However, despite numerous studies, the model seems to be not yet completely understood.

In this Letter, we shall deal with the thermal stability of a droplet of minority spins in the two–dimensional Ising model with *fixed magnetization*, monitoring the transition from a compact single, macroscopic and extensive droplet at low temperatures to an ensemble of small clusters at high temperatures. Although related cluster equilibrium properties have been studied rather carefully in the usual, *grand–canonical* Ising model [2, 3], this topic seems to have been largely overlooked. Only recently, the corresponding thermal behaviour of an adatom or vacancy island of monoatomic height on a crystal surface has been investigated [4].

In particular, we consider a square lattice with L^2 sites and full periodic boundary conditions. Neighbouring spins, $S_{i(j)} = \pm 1$, may interact ferromagnetically, with the coupling term $-JS_iS_j$, $J > 0$. We assume that N^2, out of totally L^2, spins are '$-$' spins, with the magnetization

$$M = 1 - 2(N^2/L^2) \tag{1}$$

being conserved when varying the temperature, T.

The resulting phase diagram in the (M, T)–plane is known to display a transition of first order between droplet and stripe phases [5, 6, 7]. The transition takes place in the coexistence region, which is bounded by $T_0(M_0)$ describing the temperature dependence of the spontaneous magnetization of the standard Ising model. In the thermodynamic limit, M_0 is determined by [1]

$$M_0 = \left[1 - (\sinh 2J/(k_BT_0))^{-4}\right]^{1/8}. \tag{2}$$

Another intriguing feature of the droplet phase in the coexistence region, $T < T_0$, will be discussed in the following, the thermal stability of the droplet of minority spins, i.e. '$-$' spins for $M > 0$.

At $M > 1/2$, the N^2 minority spins form a single square droplet in the ground state. When increasing the temperature at fixed magnetization, the largest cluster will, of course, shrink, but it may be, at sufficiently low temperatures, still extensive, with the number of cluster spins, thermally averaged, $< N_c >$, being proportional to L^2 ($\propto N^2$). Accordingly, the droplet size n_c defined by

$$n_c = < N_c > /N^2, \tag{3}$$

will be non–zero in the thermodynamic limit, $L, N \longrightarrow \infty$, with M (N/L) being constant.

However, at and above the coexistence line, $T > T_0$, the largest cluster is expected
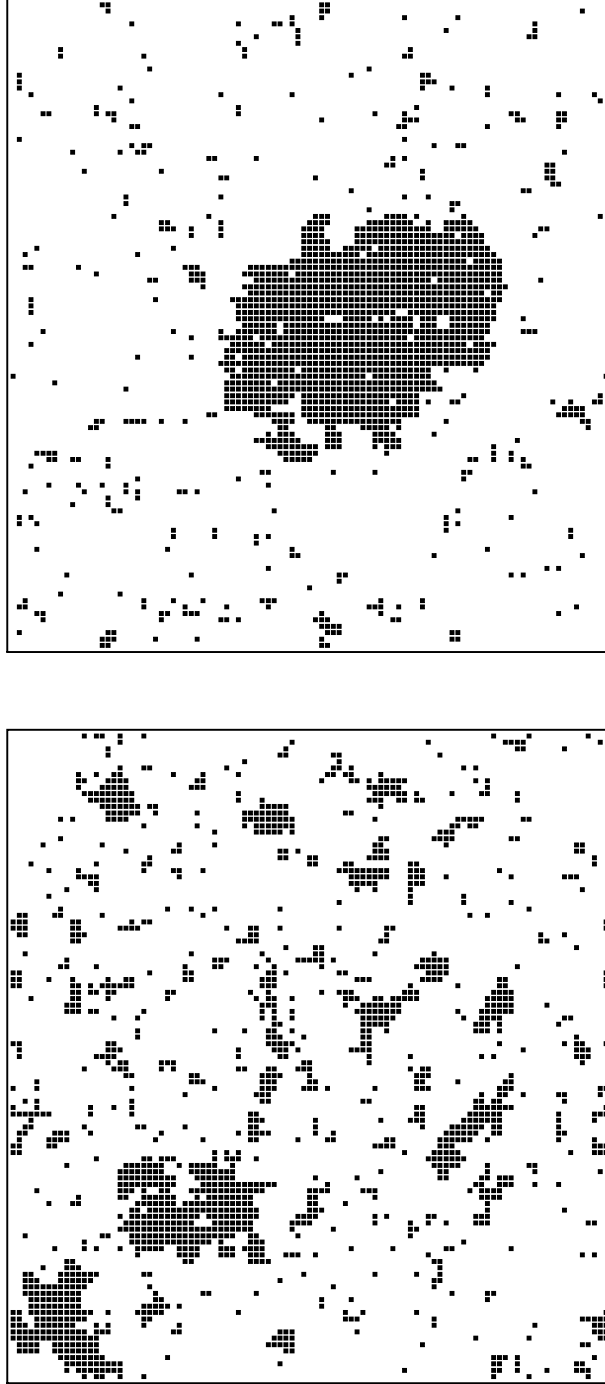
Figure 1. Typical equilibrium configurations of the two–dimensional Ising model, at $M = 0.68$, below (a: $k_BT/J = 2$) and above (b: $k_BT/J = 2.25$) the cluster transition, simulating a lattice with 100^2 sites; '$-$' spins are denoted by dark squares.

to be non–extensive [2], see Fig. 1. Thence, one expects a 'cluster transition', T_{cl} at or below T_0. Indeed, assuming that, in the coexistence region, see Ref. 8,

$$-M_d = M_s = M_0 \tag{4}$$

where M_d is the magnetization in the droplet, M_s is the magnetization in the rest of the system, and M_0 is given by Equation (2), one may easily obtain $n_c(T)$, at fixed magnetization M, as

$$n_c(T) = (1 + M_0)(M_0 - M)/(2M_0(1 - M)) \tag{5}$$

Obviously, the droplet size will then vanish linearly in the reduced temperature $t = |T_0 - T|/T_0$ as $T \longrightarrow T_0$ [9].

To investigate the cluster transition and to check this relation, we did Monte Carlo simulations using a nonlocal spin-exchange algorithm [10] as well as an efficient cluster algorithm [11], studying square lattices of various sizes, L^2, with L ranging from 25 to 950, at various magnetizations M, ranging from 0.68 to 0.98.

As illustrated in Fig. 2, the droplet size $n_c(M, L, T)$ seems to approach Equation (5), as one considers larger and larger lattices, being presumably valid in the thermodynamic limit, $L, N \longrightarrow \infty$. This behaviour holds at all values of M, we studied. In addition, one observes rather interesting finite–size effects.

First, the cluster transition is signalled, in a finite system, by the turning point of $n_c(T)$, at $T_s(L)$. For moderate system sizes, with L up to, say, 750, $T_s(L)$ is found to vary (almost) linearly in $1/L$, for different values of M. A straightforward linear extrapolation would yield cluster transition temperatures close to, but somewhat below T_0. Accordingly, one may expect subtle finite–size corrections to the observed linear behaviour.– In this context, attention is drawn to the non–monotonic size dependence of $n_c(T)$ close to the coexistence temperature T_0, see Fig. 2. Obviously, rather large systems need to be considered in the vicinity of T_0 to allow a reliable extrapolation to the thermodynamic limit.

Another interesting finite–size effect is found by studying the size dependence of the largest cluster $< N_c >$ close to T_0. For small lattices, the droplet size scales like L^x, with the (effective [12]) exponent x, at fixed temperature, being quite small, e.g. at $M = 0.92$ x is seen to be around 0.5 to 0.7. Only for larger lattices, the cluster seems to become more compact, with $x \approx 2$. The crossover, at L_c, is characterised by a pronounced peak in the effective exponent x, with the peak height and crossover length L_c increasing as T approaches T_0. Obviously, this phenomenon is not predicted by Equation (5) which assumes a compact, extensive droplet, as seems to be correct in the thermodynamic limit.

Previous evidence for the cluster transition is rather scarce. In the context of an adatom island on a crystal surface, the related transition was noticed [4], but it was not discussed in the framework of the phase diagram of the corresponding Ising
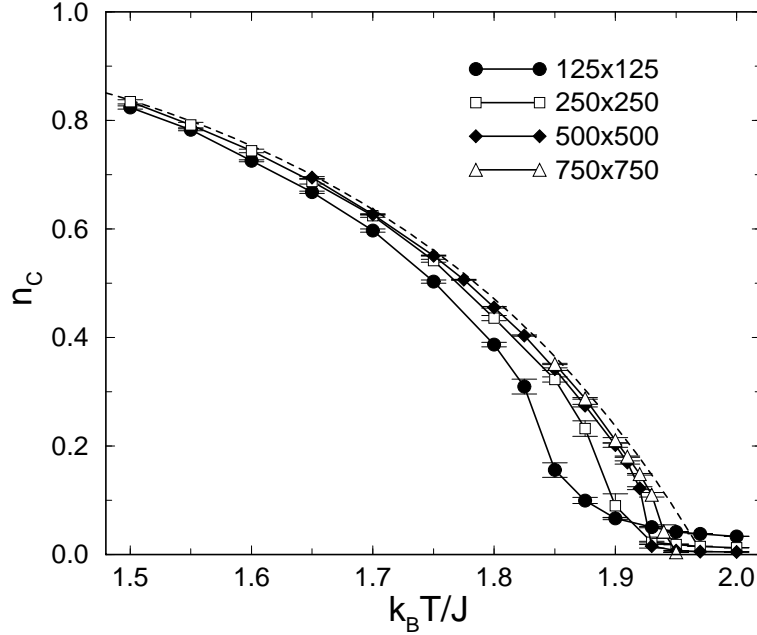
Figure 2. Droplet size n_c as function of temperature for lattice sizes L ranging from 125 to 750, at fixed magnetization $M = 0.92$. Error bars stem from averaging over at least $N = 10$ Monte Carlo runs with different random numbers. The dashed line corresponds to Equation (5).

model. In that study, a non–trivial critical exponent describing the vanishing of the droplet size n_c on approach to the cluster transition had been obtained, estimating the transition temperature from a straightforward linear extrapolation of simulational data for moderate system sizes, as discussed above.– A possible hint on the cluster transition might be hidden in a renormalization group study of Saito [13] on quenches in Ising models with conserved magnetization, finding, however, a transition below the coexistence line, without mentioning of the thermal stability of the droplet.– Attention is also drawn to the work of Kertész on droplet stability in Ising models in an external field [14] as well as related recent work on Ising cubes [15, 16] and cluster shapes [8].

It looks quite promising to analyse various cluster properties close to the cluster transition, in analogy to percolation studies [3]. For instance, we find that the second moment of the cluster size distribution, excluding the largest cluster, shows a pronounced peak close to T_s, indicating a divergence at the cluster transition in the thermodynamic limit. Furthermore, the specific heat also displays a pronounced maximum close to T_s.

In summary, we conclude that there seems to be, in the two–dimensional Ising model with conserved magnetization, a cluster transition at the coexistence line, at which the droplet of minority spins looses, in the thermodynamic limit, its extensivity. We think that the interesting cluster and thermal properties as well as finite–size effects close to

that transition deserve to be studied in more detail in the future, both in two and three dimensions.

Acknowledgments

References

[1] McCoy B and Wu T T 1973 *The two–dimensional Ising model* (Cambridge: Harvard University Press)

[2] Coniglio A and Klein W 1980 *J. Phys. A: Math. Gen.* **13** 2775

[3] Stauffer D and Aharony A 1994 *Introduction to percolation theory* (London: Taylor and Francis)

[4] Müller T and Selke W 1999 *Eur. Phys. J.* B**10** 549

[5] Shlosman S B 1989 *Commun. Math. Phys.* **125** 81

[6] Leung K and Zia R K P 1990 *J. Phys. A: Math. Gen.* **23** 4593

[7] Berg B A, Hansmann U, and Neuhaus T 1993 *Phys. Rev. B* **47** 497

[8] Bodineau T, Ioffe D, and Velenik Y 2000 *J. Math. Phys.* **41** 1033

[9] van Beijeren H 1999 (private communication)

[10] Barkema G T, Newman M E J, and Breeman M 1994 *Phys. Rev. B* **50** 7946

[11] Heringa J R and Blöte H W J 1998 *Phys. Rev. E* **57** 4976

[12] Pleimling M and Selke W 1998 *Eur. Phys. J. B* **1** 385

[13] Saito Y 1978 *Prog. Theor. Phys.* **59** 375

[14] Kertész J 1989 *Physica* A**161** 58

[15] Carmona J M, Richert J, and Tarancón A 1998 *Nucl. Phys.* A**643** 115

[16] Gulminelli F and Chomaz Ph 1999 *Phys. Rev. Lett.* **82** 1402